Phenanthrene, 9-methyl-

Other names: 9-Methylphenanthrene
Inchi: InChI=1S/C15H12/c1-11-10-12-6-2-3-8-14(12)15-9-5-4-7-13(11)15/h2-10H,1H3
InchiKey: DALBHIYZSZZWBS-UHFFFAOYSA-N
Formula: C15H12
SMILES: Cc1cc2ccccc2c2ccccc12
Mol. weight [g/mol]: 192.26
CAS: 883-20-5

Physical Properties

Property code	Value	Unit	Source
gf	381.87	kJ/mol	Joback Method
hf	242.80	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
ie	7.46 ± 0.03	eV	NIST Webbook
log10ws	-5.56		Crippen Method
logp	4.301		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	319.20		NIST Webbook
rinpol	322.65		NIST Webbook
rinpol	323.06		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.92		NIST Webbook
rinpol	322.78		NIST Webbook
rinpol	323.28		NIST Webbook
rinpol	324.71		NIST Webbook
rinpol	322.61		NIST Webbook
rinpol	323.24		NIST Webbook
rinpol	322.90		NIST Webbook
rinpol	323.10		NIST Webbook
rinpol	322.86		NIST Webbook
rinpol	322.81		NIST Webbook
rinpol	323.06		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.74		NIST Webbook
rinpol	322.78		NIST Webbook

rinpol	322.90		NIST Webbook
rinpol	319.20		NIST Webbook
rinpol	323.10		NIST Webbook
rinpol	322.80		NIST Webbook
rinpol	323.10		NIST Webbook
rinpol	322.80		NIST Webbook
rinpol	323.30		NIST Webbook
rinpol	319.17		NIST Webbook
rinpol	323.06		NIST Webbook
rinpol	323.78		NIST Webbook
rinpol	323.06		NIST Webbook
rinpol	323.06		NIST Webbook
rinpol	322.65		NIST Webbook
rinpol	323.28		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	322.74		NIST Webbook
rinpol	323.10		NIST Webbook
tb	617.20	K	Joback Method
tc	866.35	K	Joback Method
tf	375.67	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	617.20	Joback Method
cpg	396.50	J/mol×K	658.73	Joback Method
cpg	410.54	J/mol×K	700.25	Joback Method
cpg	423.46	J/mol×K	741.78	Joback Method
cpg	435.41	J/mol×K	783.30	Joback Method
cpg	446.52	J/mol×K	824.83	Joback Method
cpg	456.90	J/mol×K	866.35	Joback Method
dvisc	0.0013574	Pa×s	375.67	Joback Method
dvisc	0.0010334	Pa×s	415.93	Joback Method
dvisc	0.0008255	Pa×s	456.18	Joback Method
dvisc	0.0006839	Pa×s	496.44	Joback Method
dvisc	0.0005828	Pa×s	536.69	Joback Method
dvisc	0.0005079	Pa×s	576.95	Joback Method
dvisc	0.0004506	Pa×s	617.20	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C883205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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